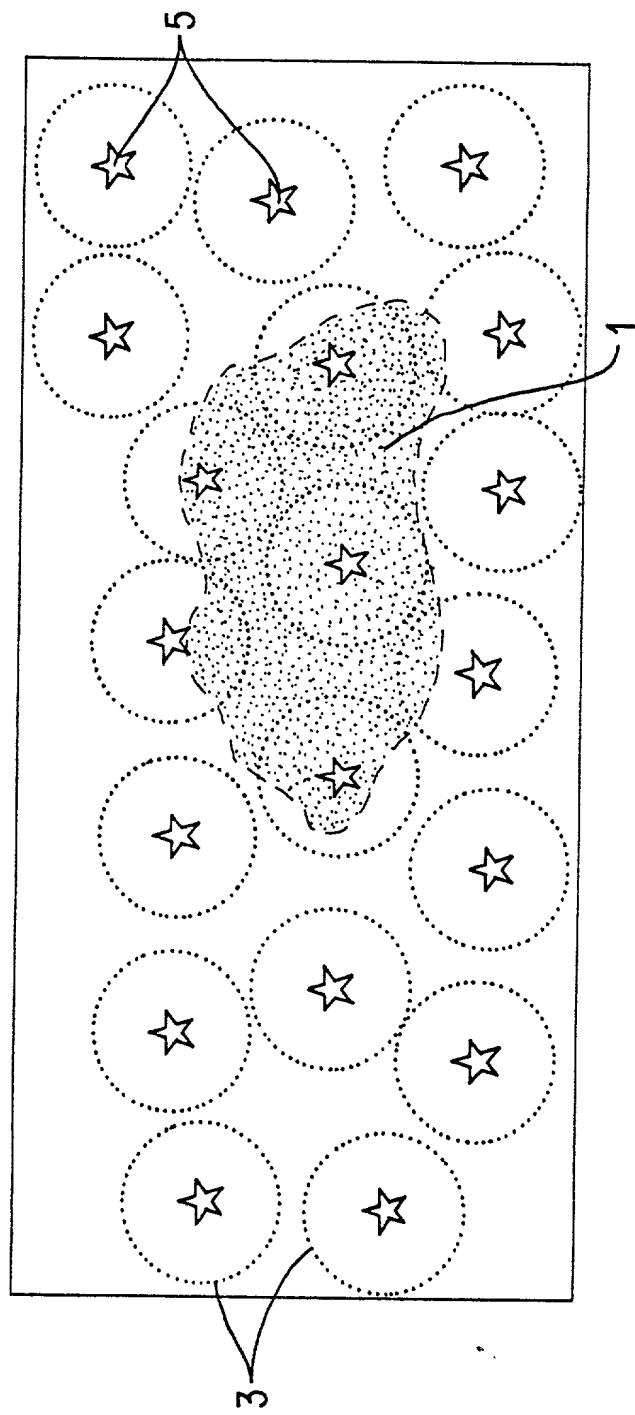


FIG. 1(a)

FIG. 1(b)



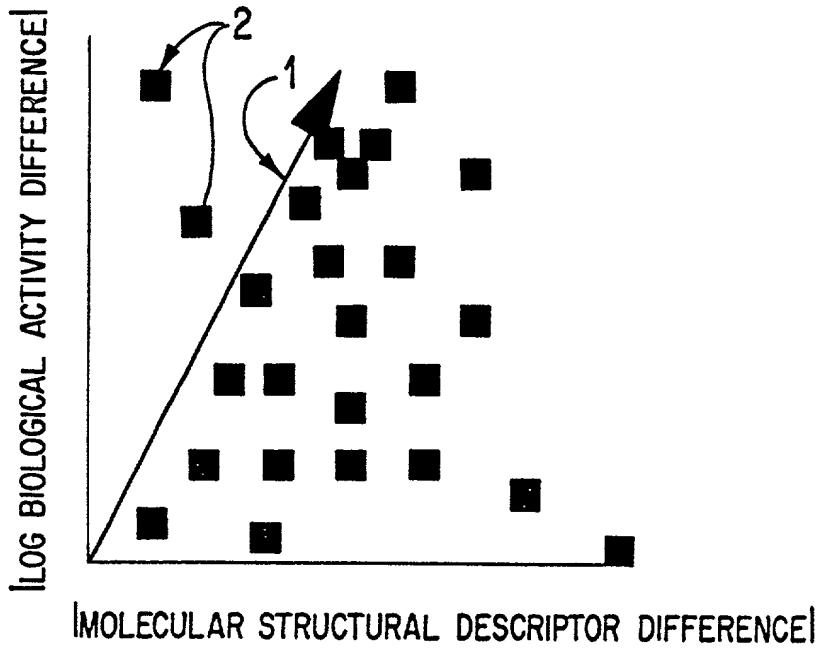


FIG. 2

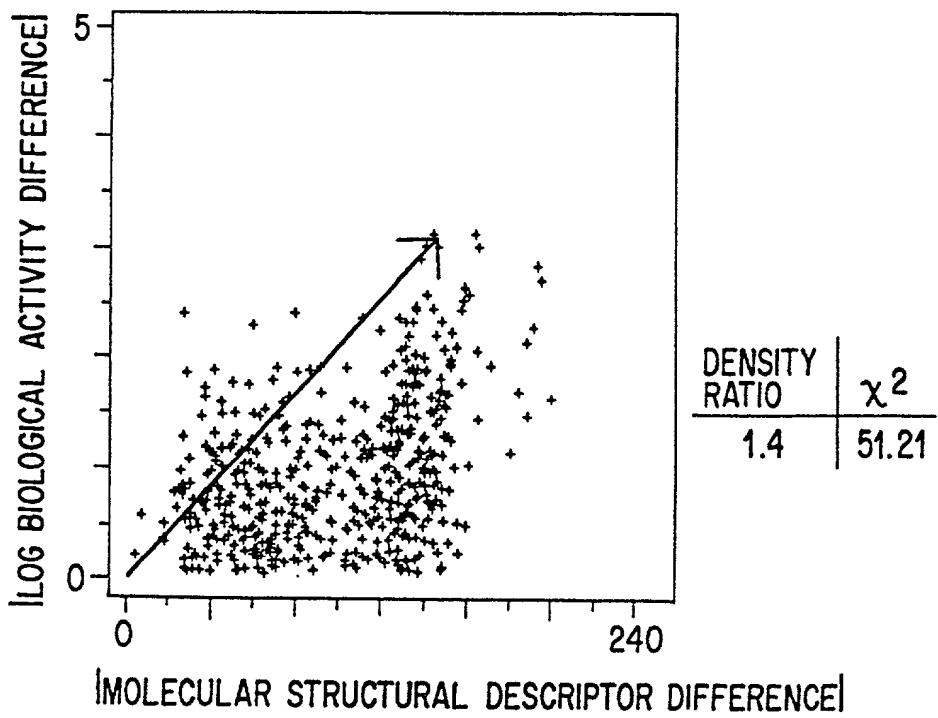


FIG. 3

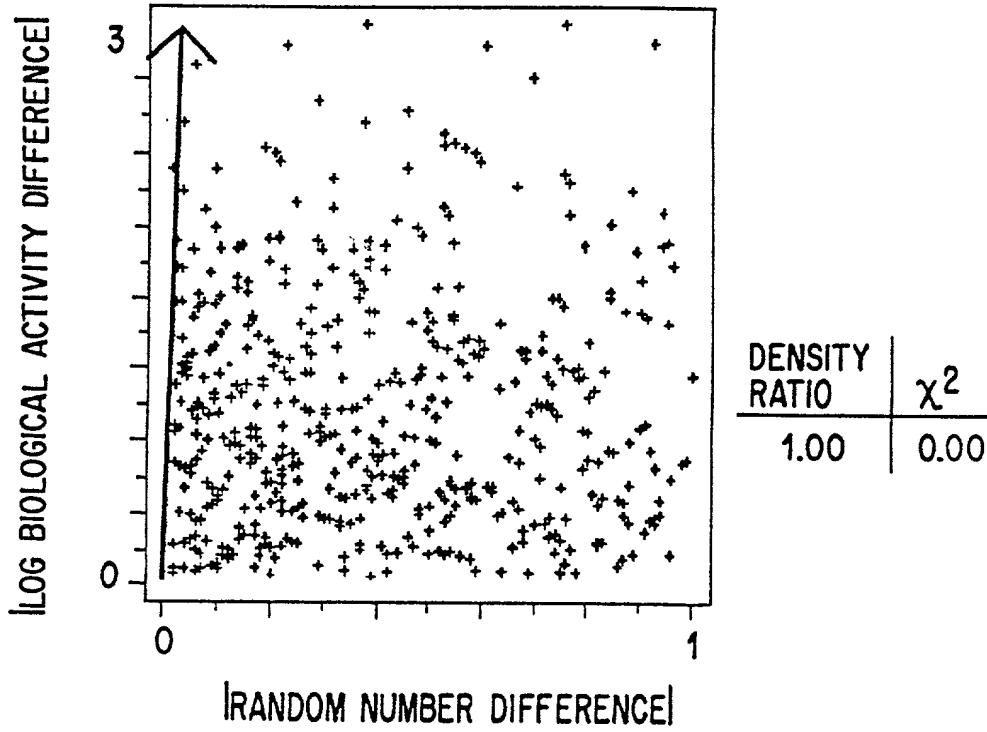


FIG. 4

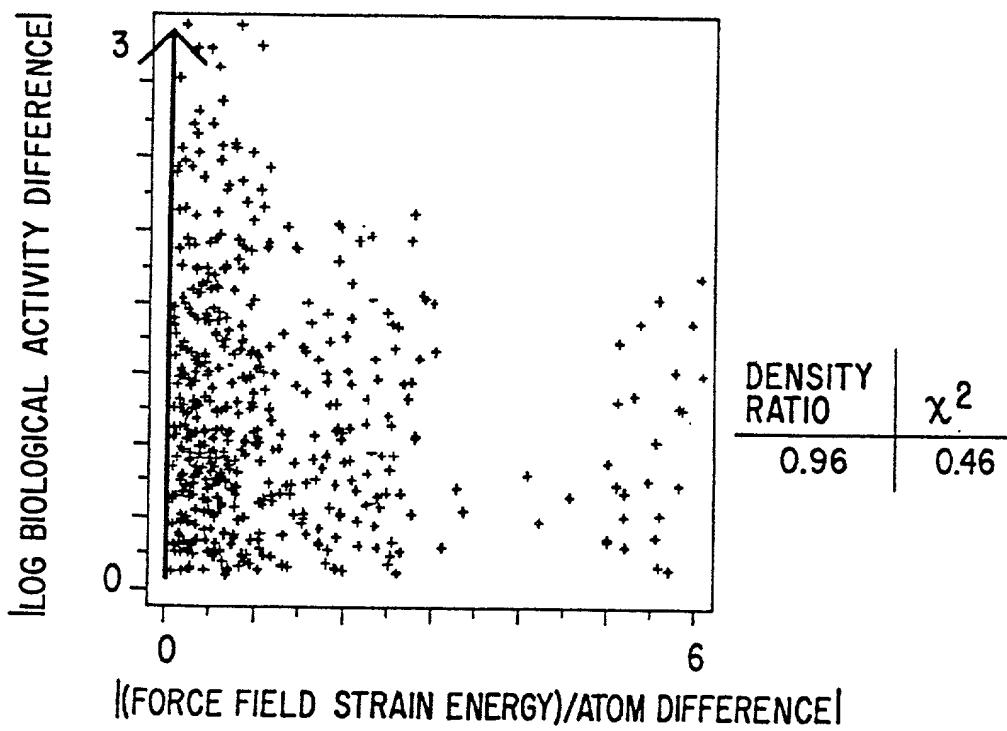
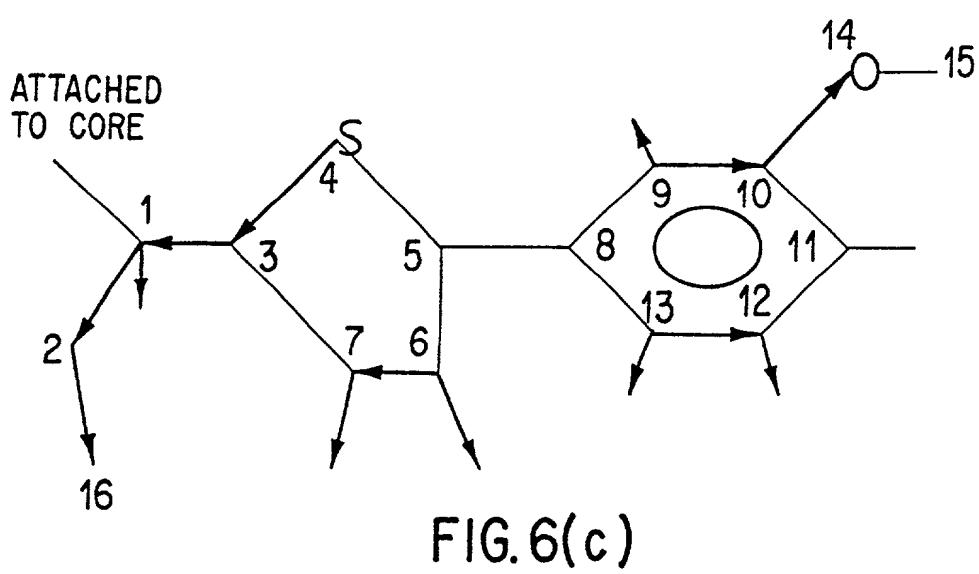
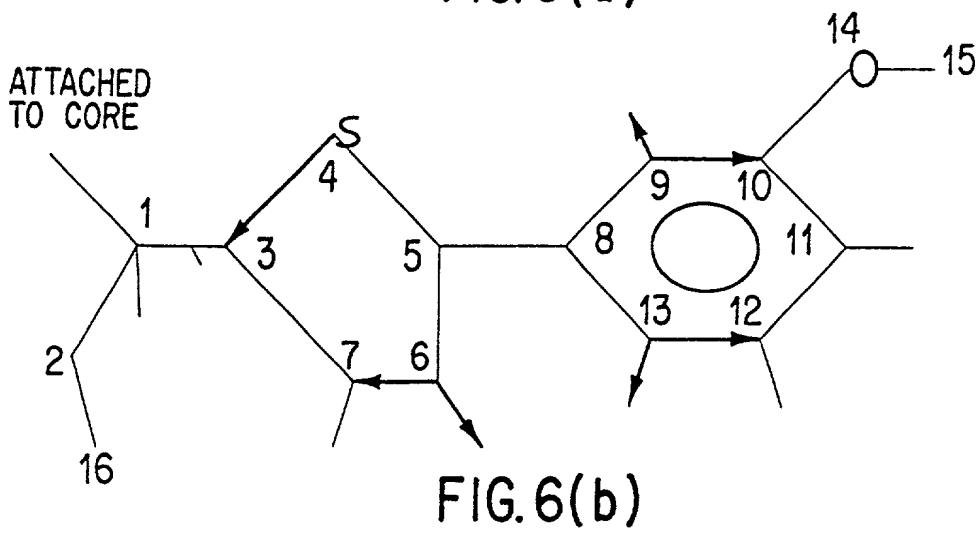
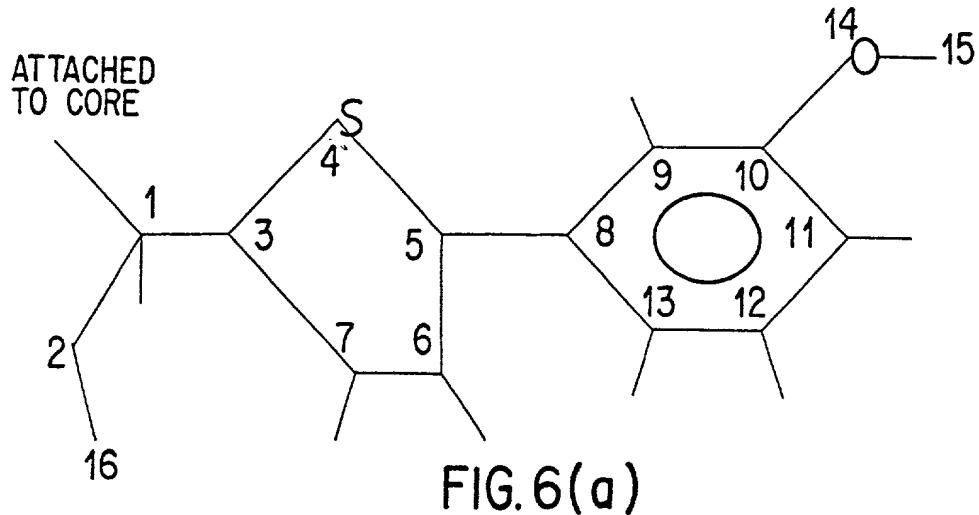


FIG. 5



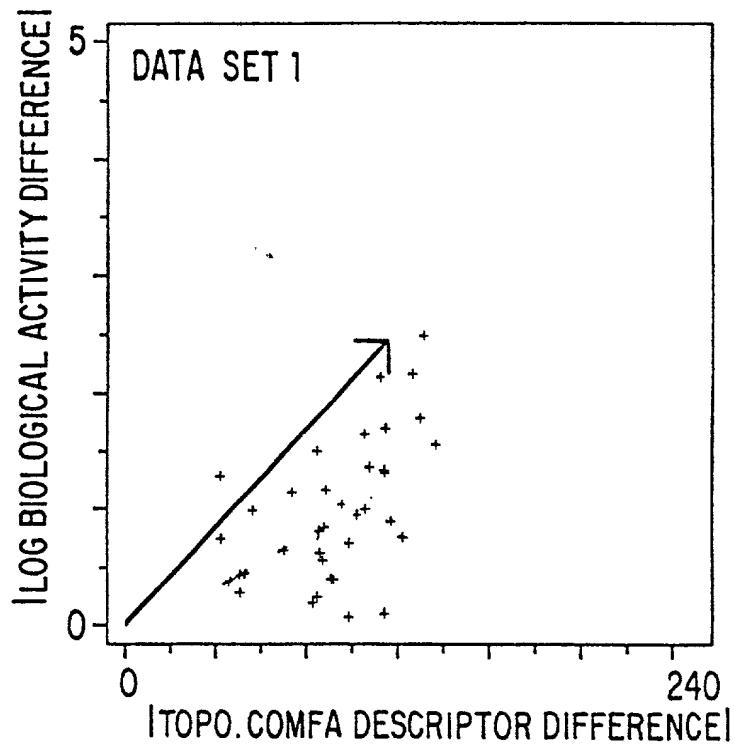


FIG.7(a)

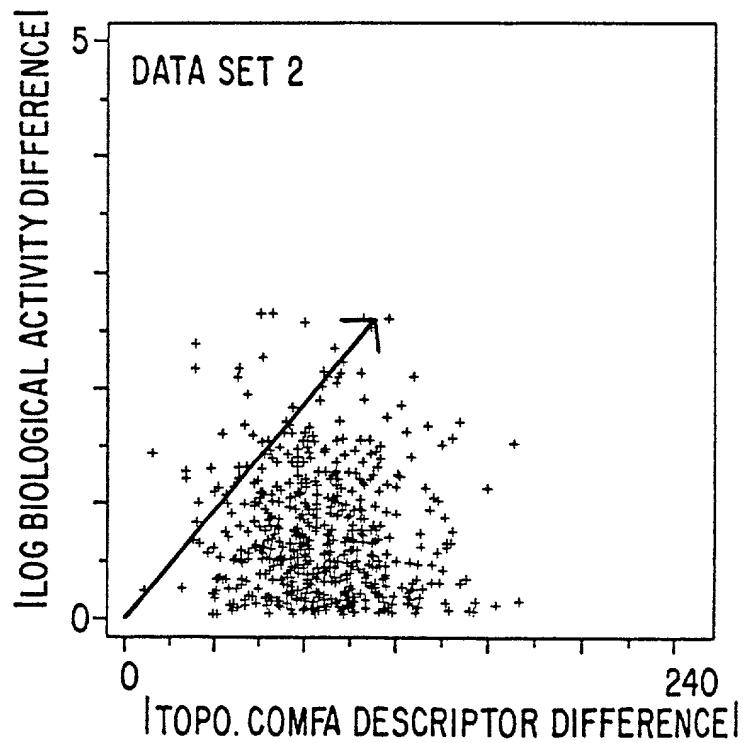


FIG.7(b)

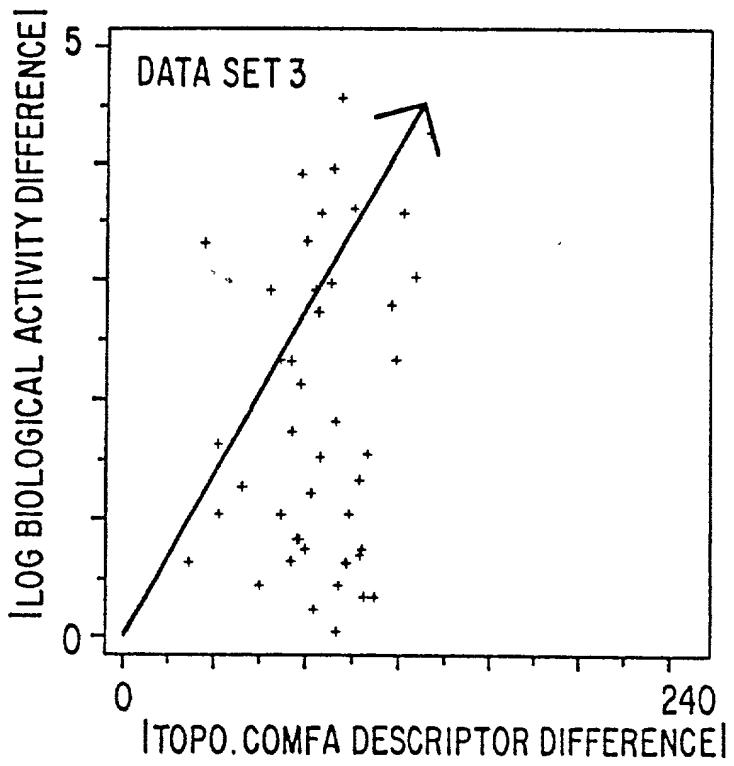


FIG. 7(c)

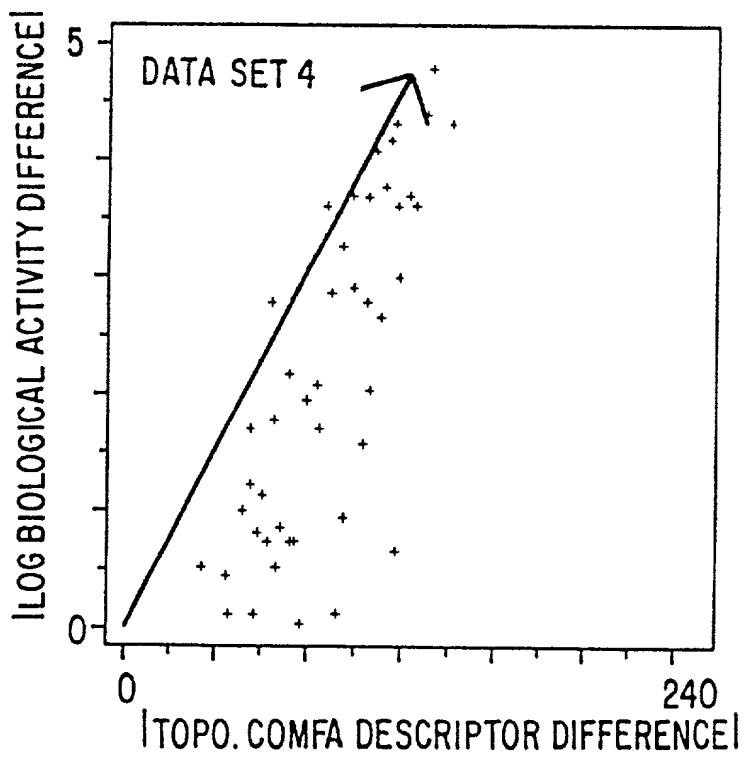


FIG. 7(d)

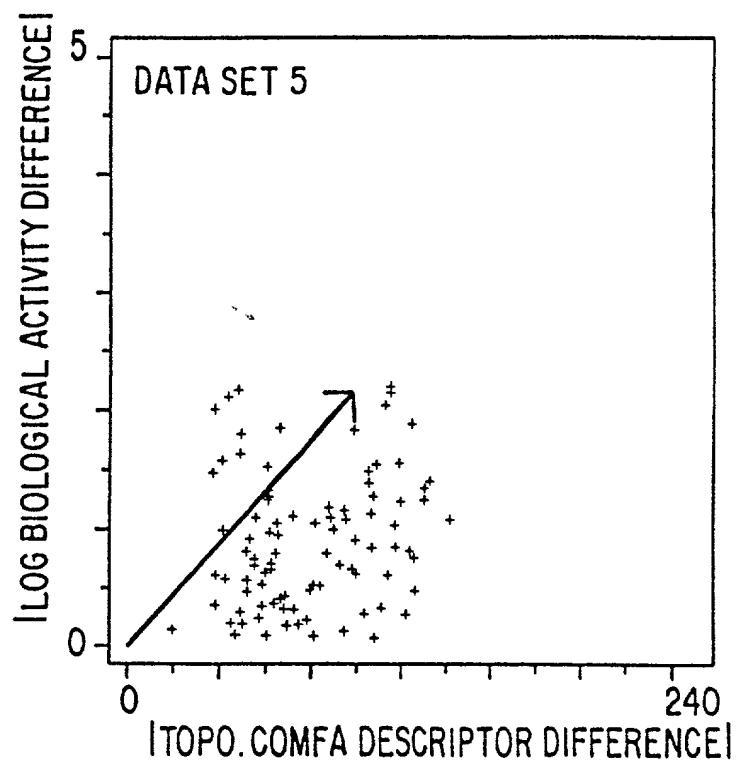


FIG.7(e)

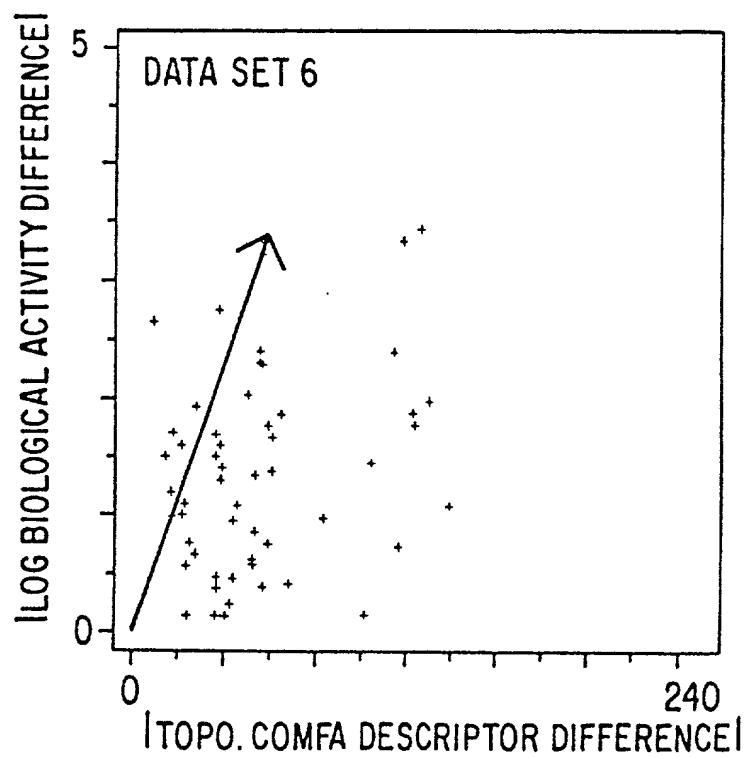


FIG.7(f)

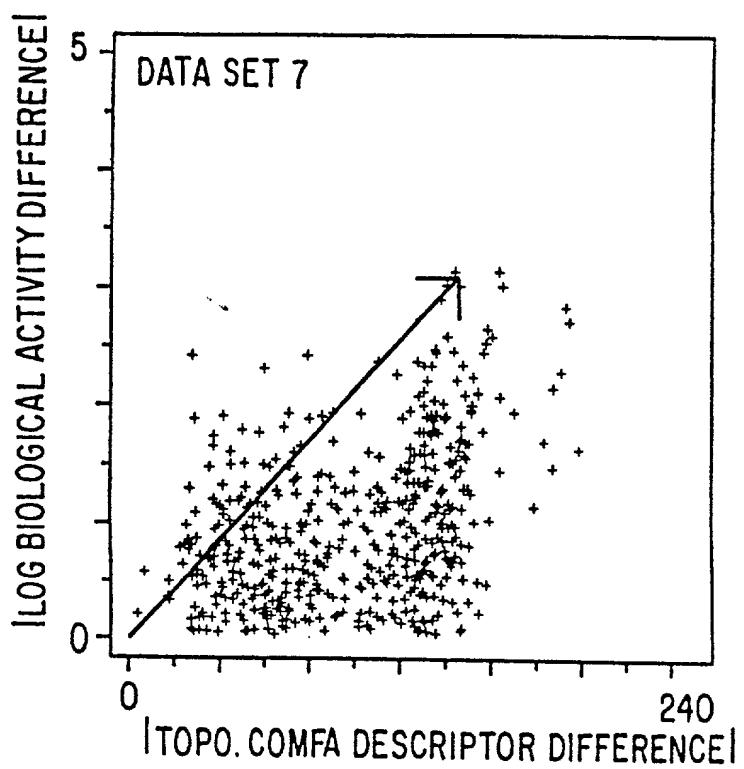


FIG.7(g)

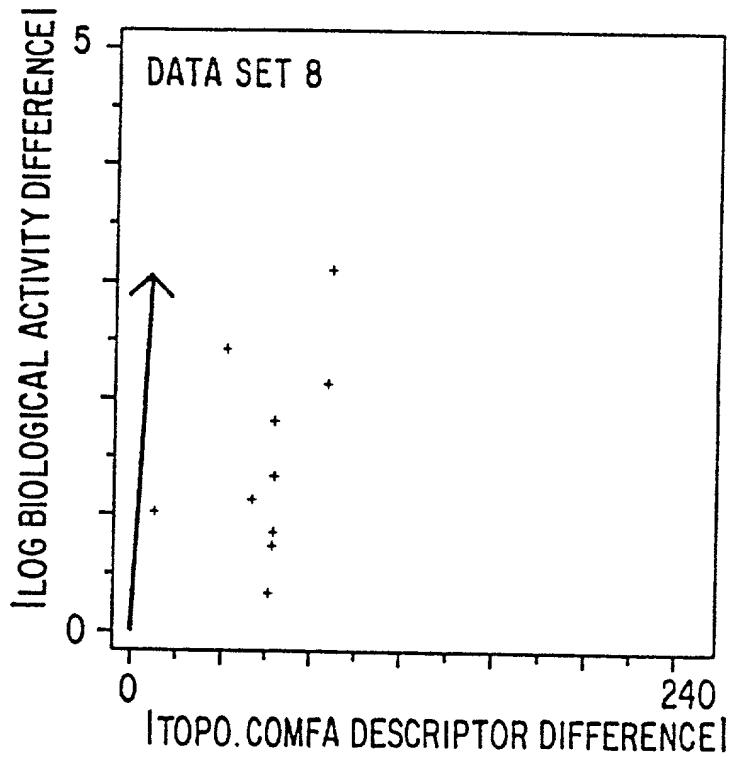


FIG.7(h)

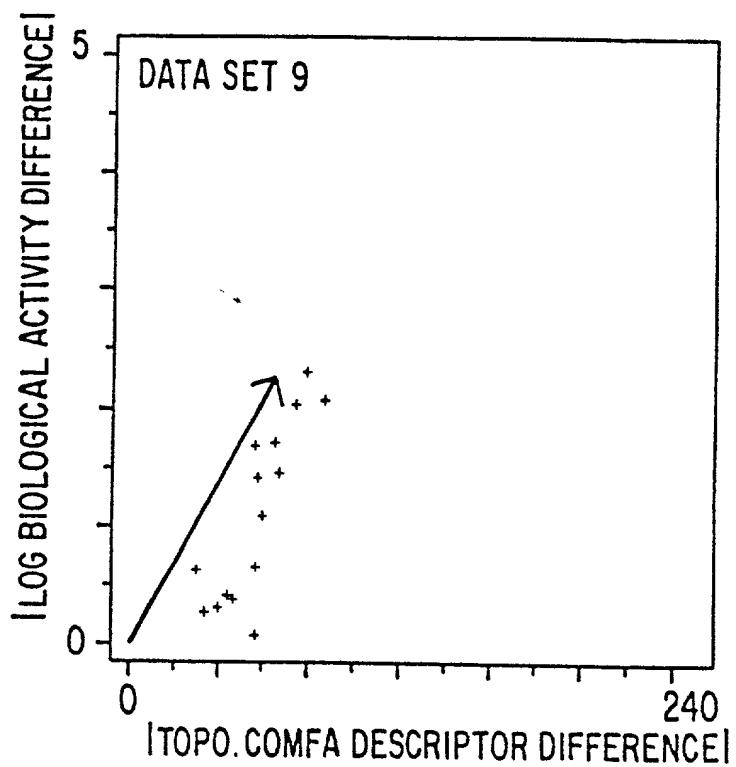


FIG.7(i)

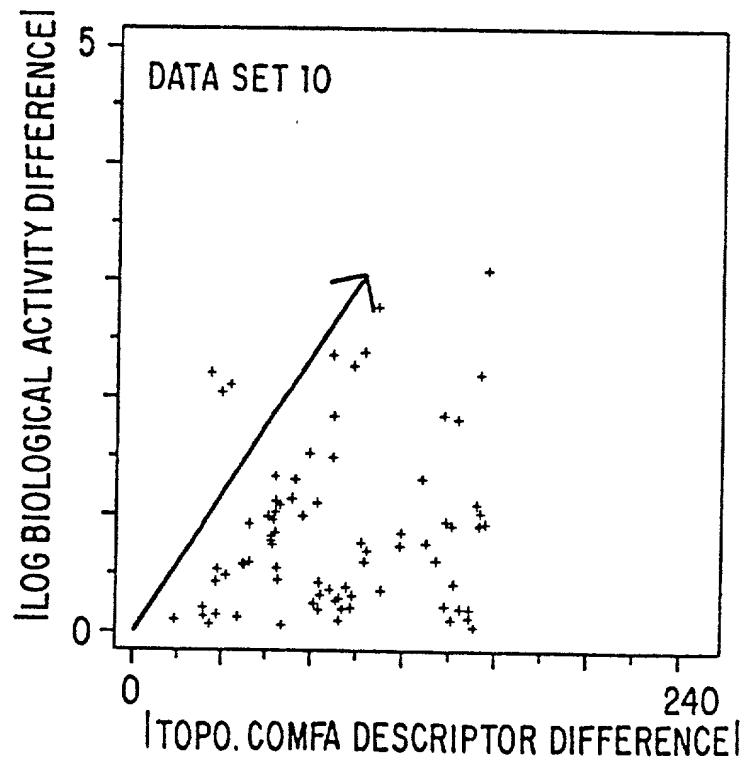


FIG.7(j)

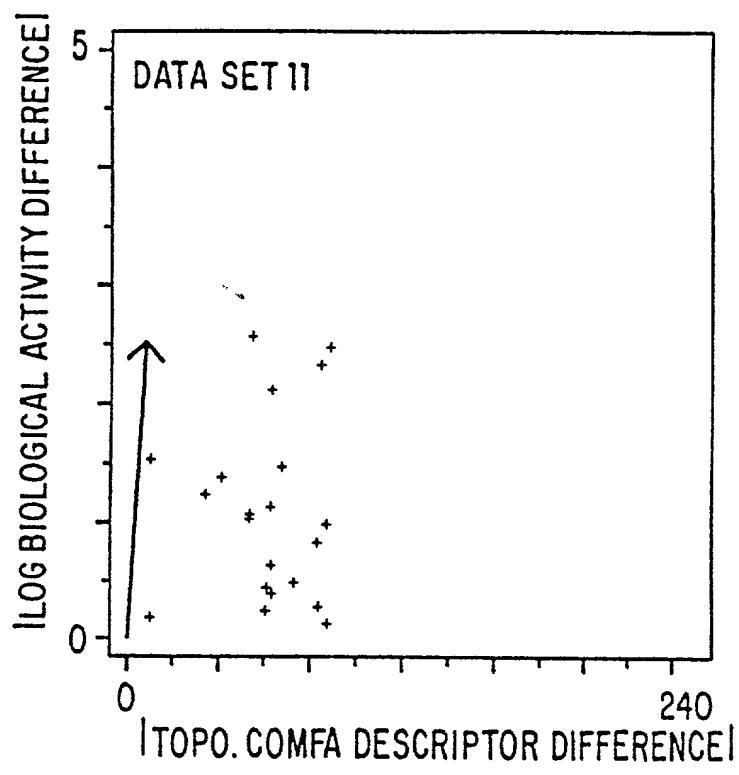


FIG.7(k)

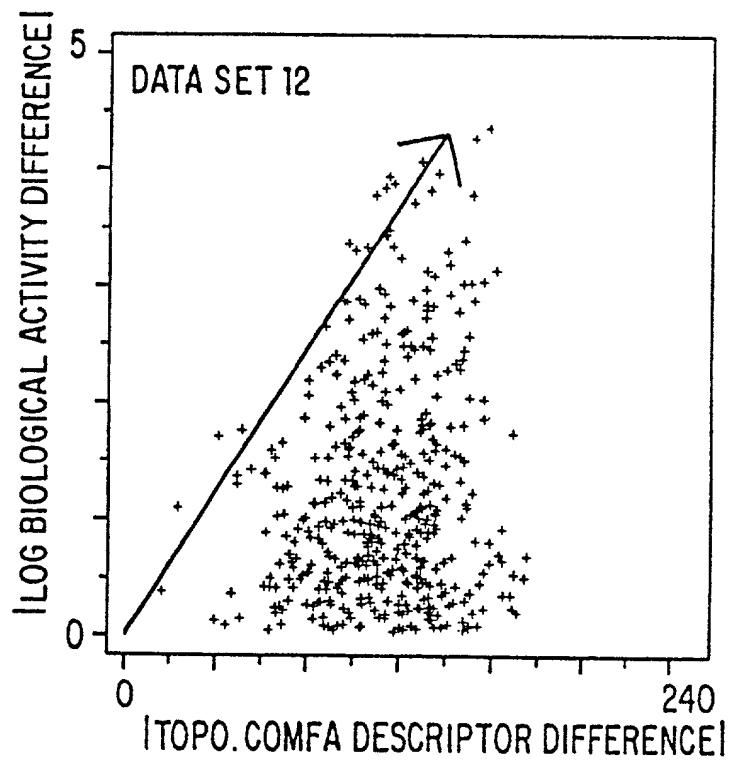


FIG.7(l)

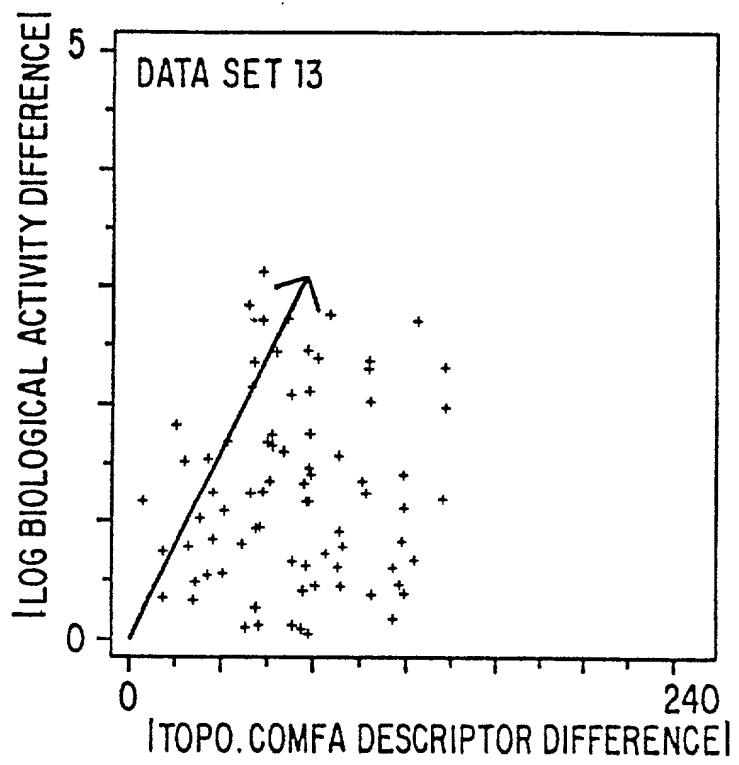


FIG.7(m)

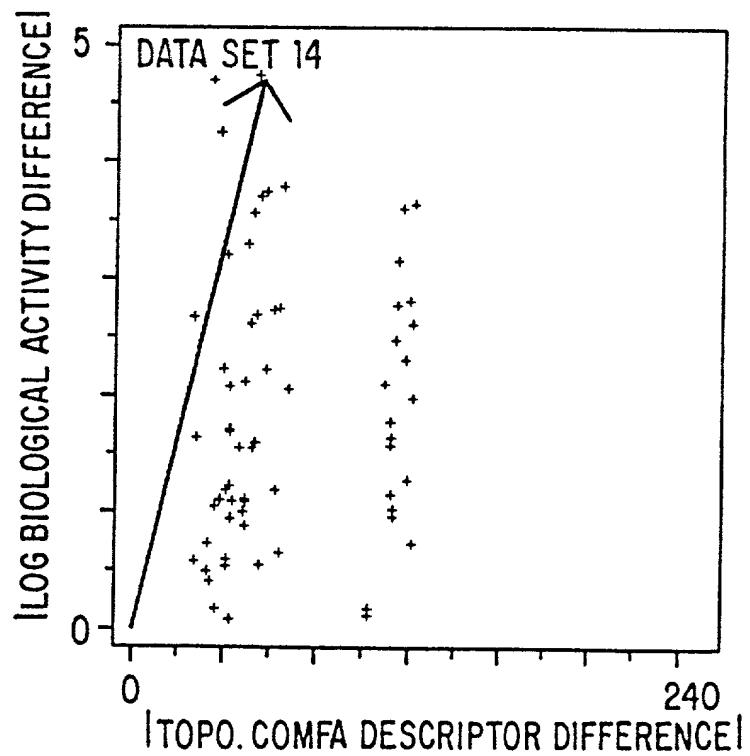


FIG.7(n)

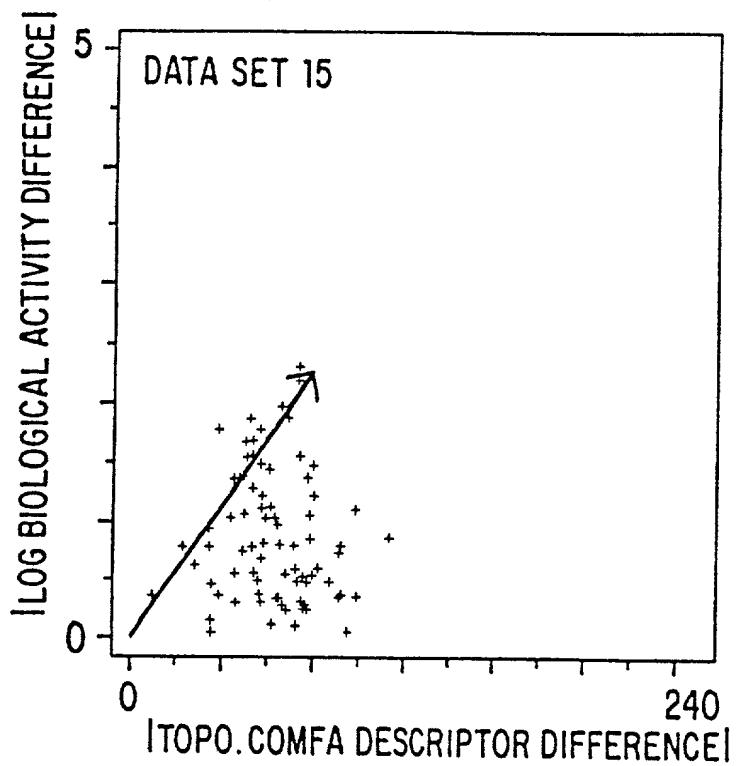


FIG.7(o)

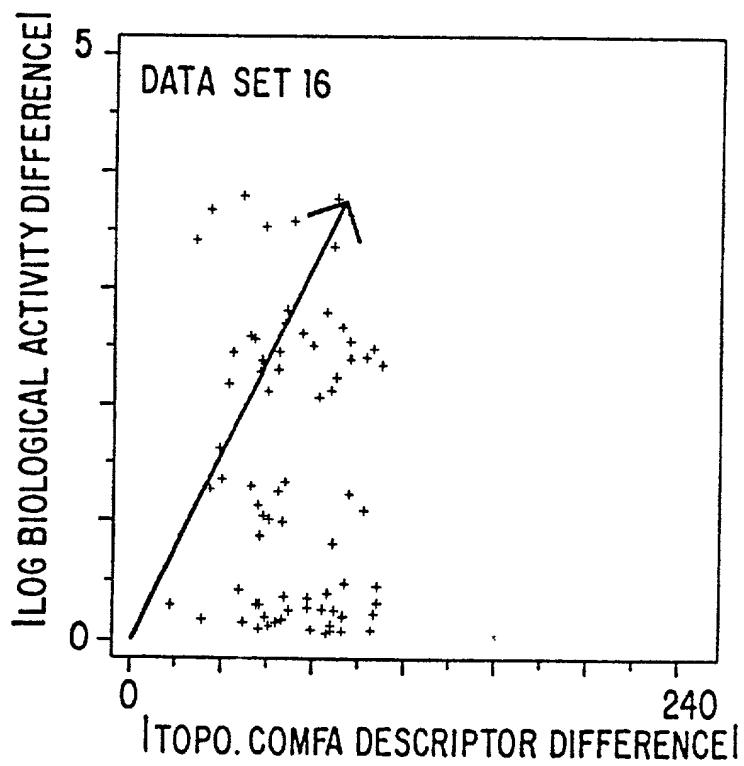


FIG.7(p)

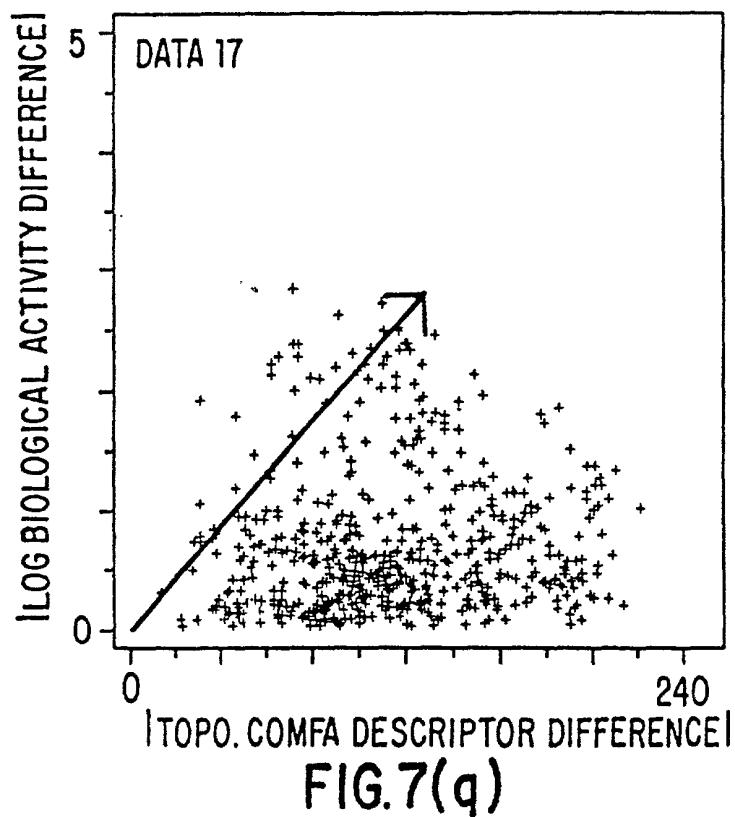


FIG.7(q)

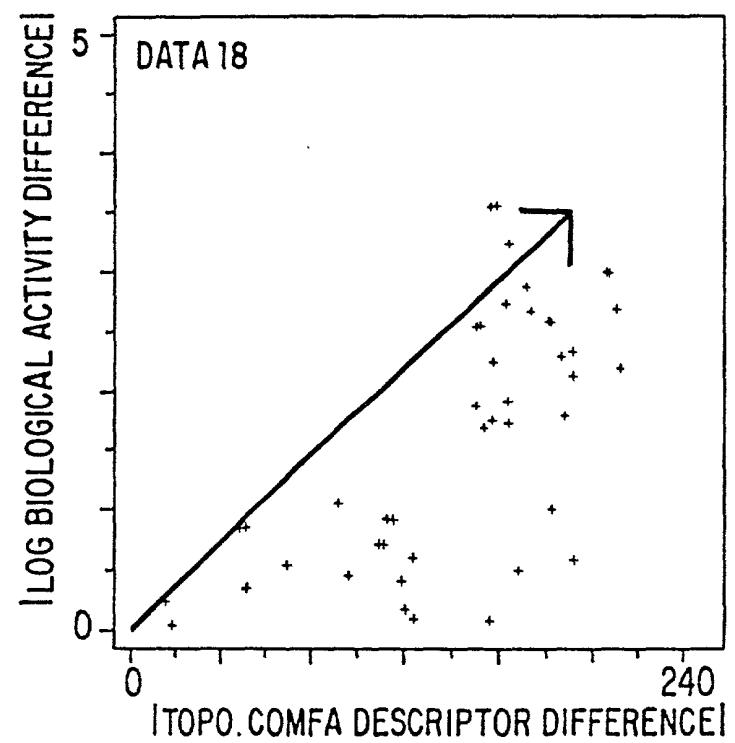


FIG.7(r)

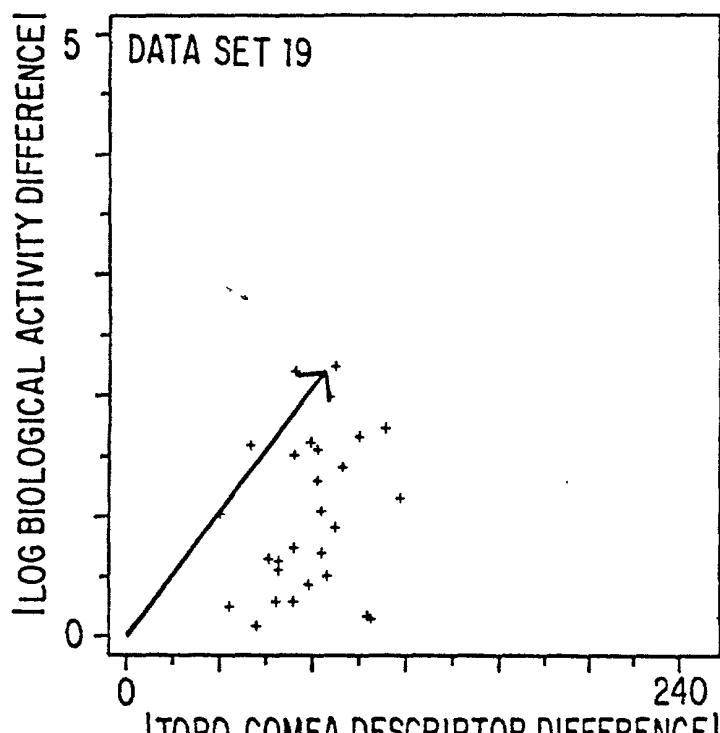


FIG.7(s)

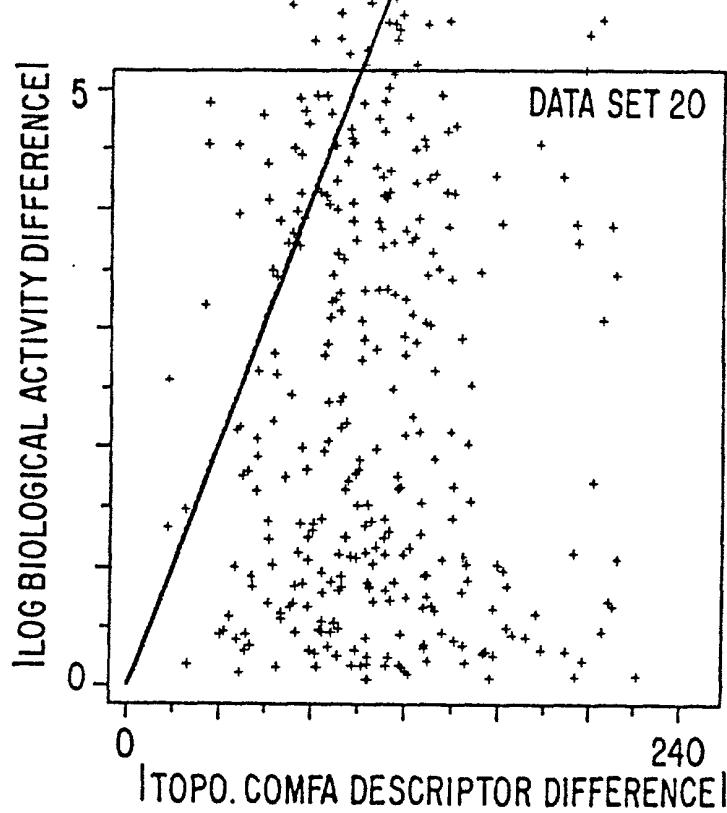
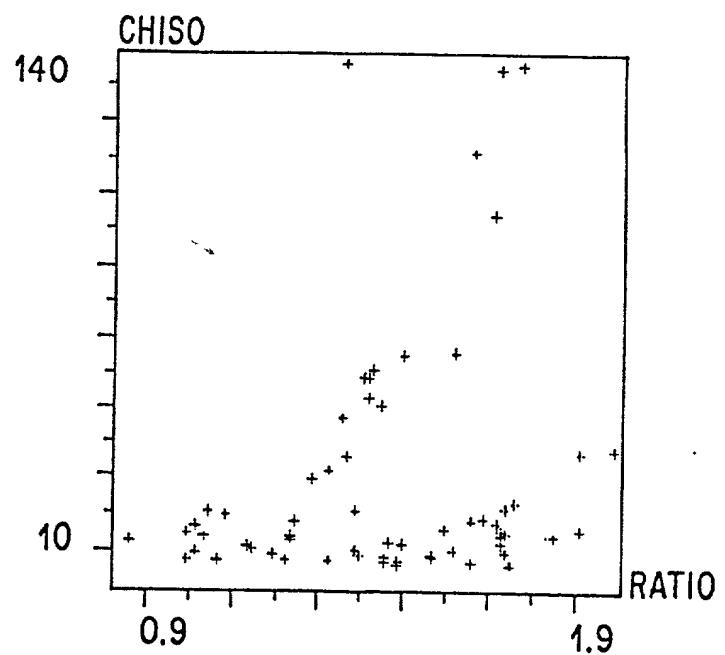
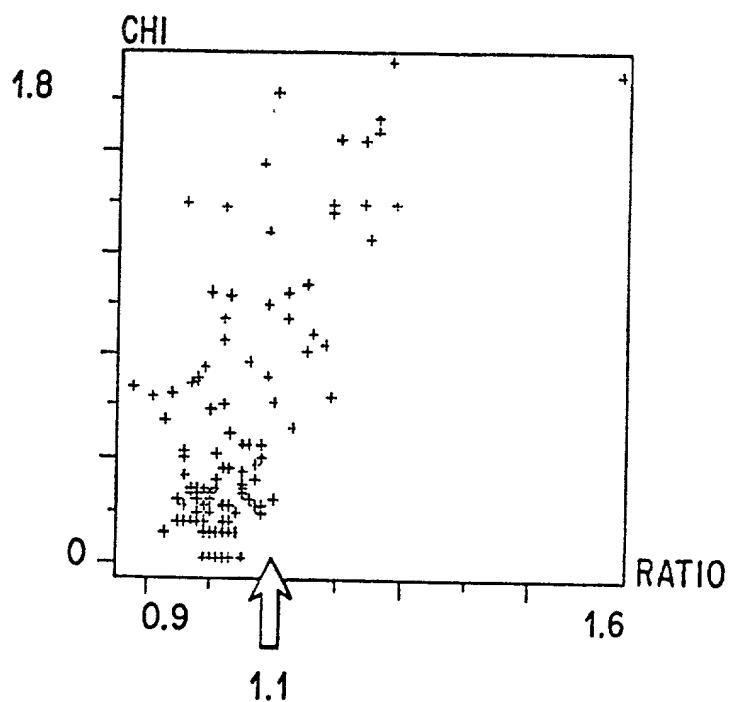


FIG.7(†)



↑
1.1

FIG. 8(a)



↑
1.1

FIG. 8(b)

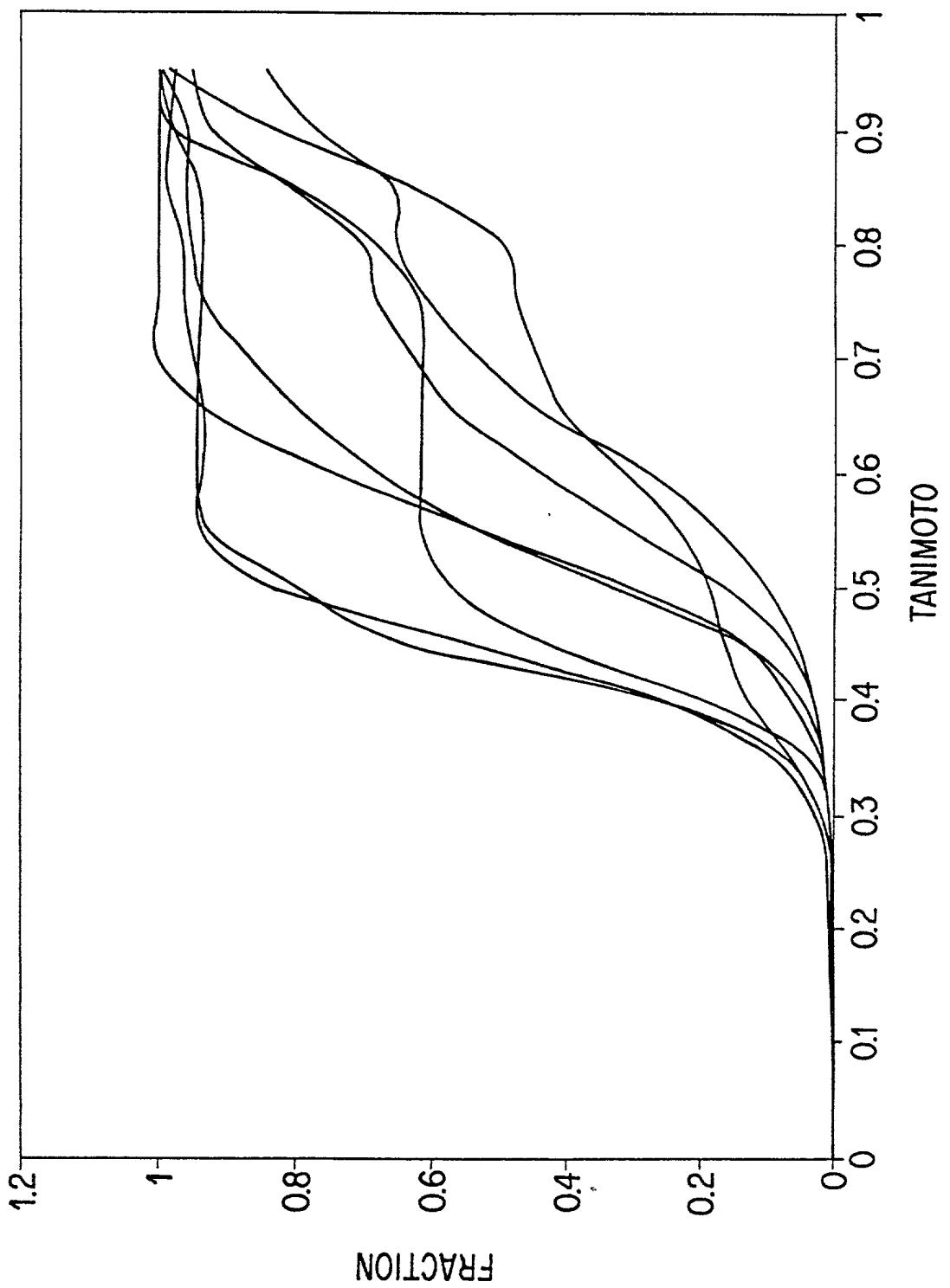


FIG. 9(a)

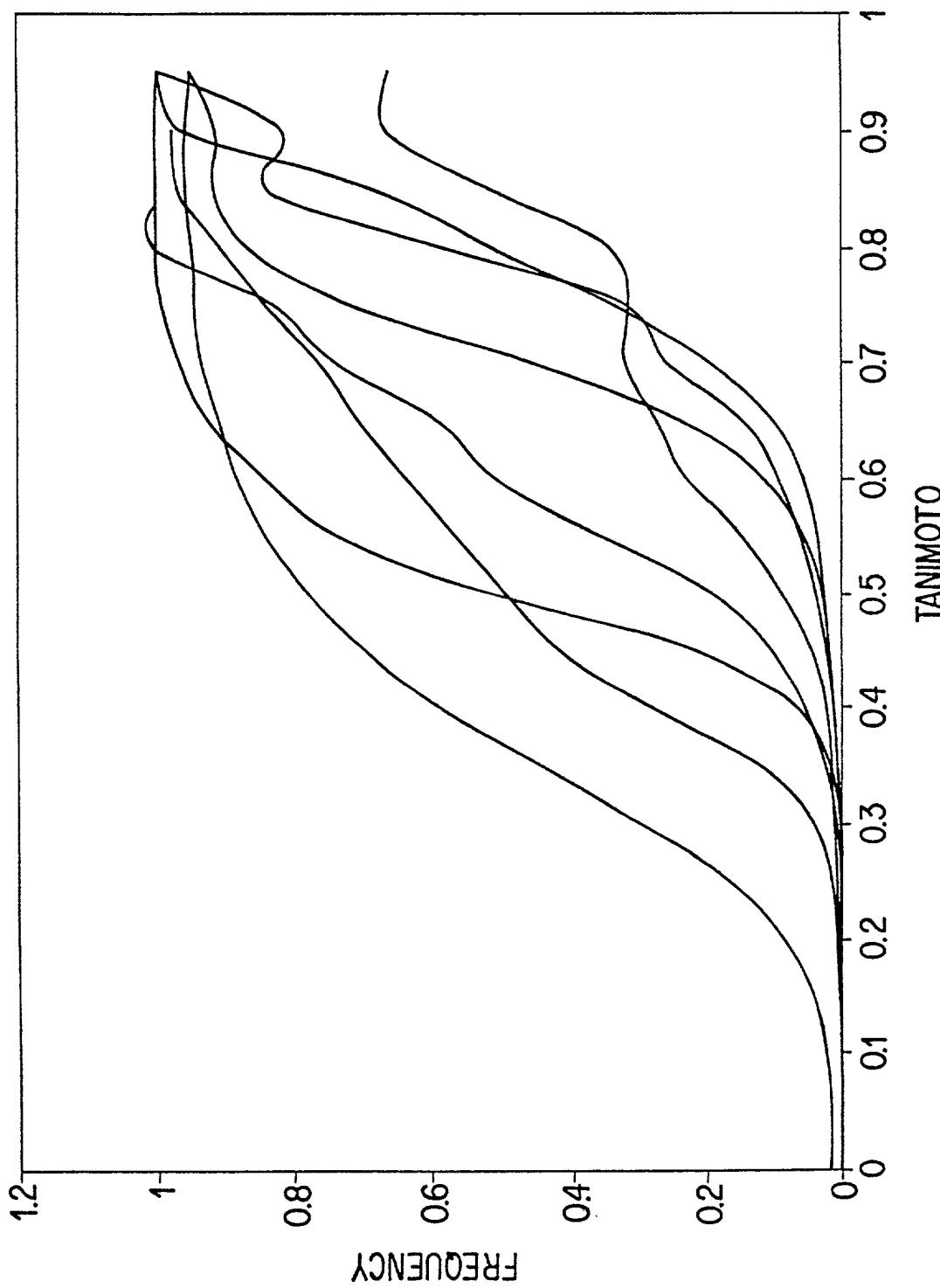
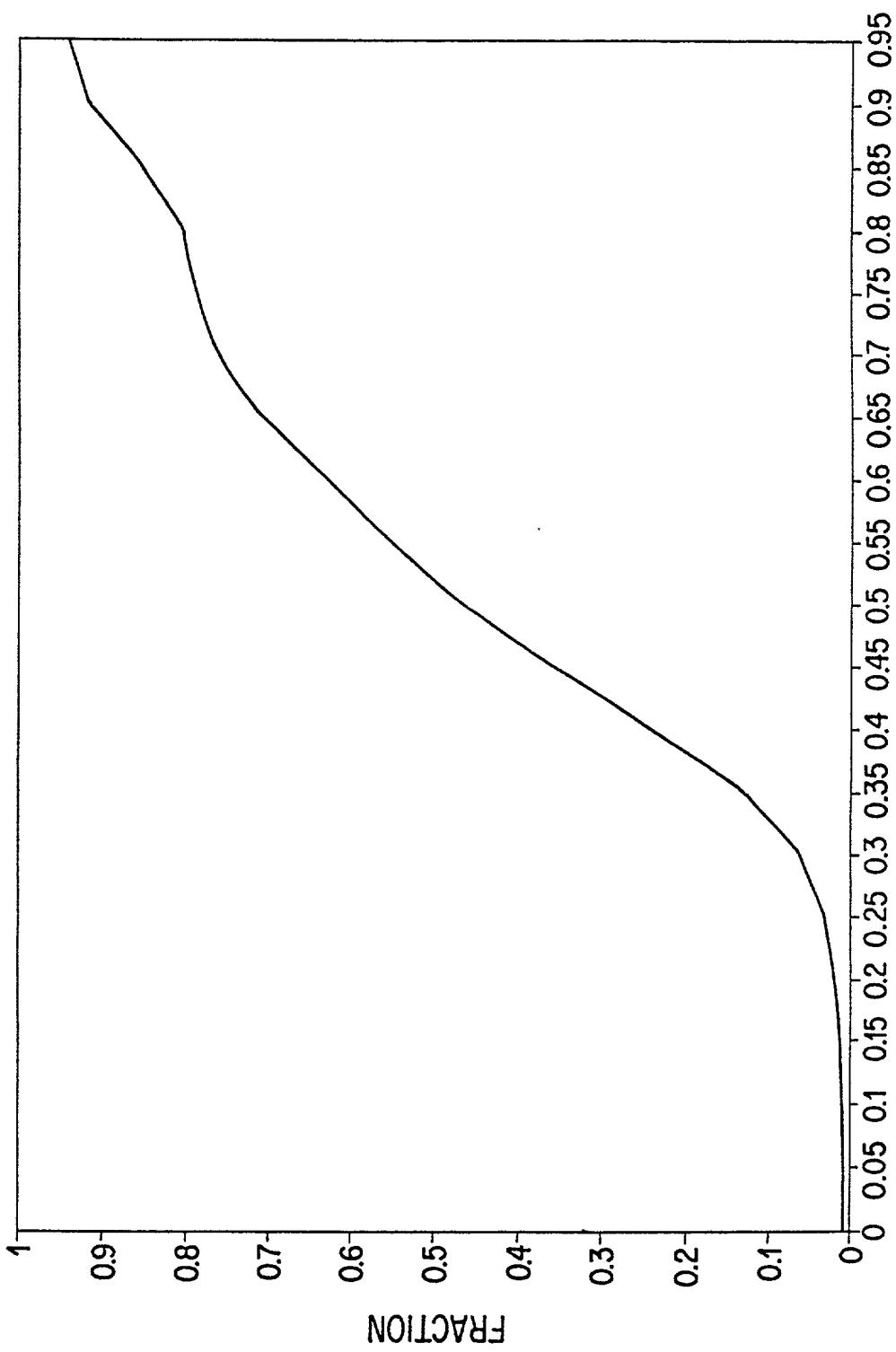


FIG. 9(b)

FIG. 9(c)

TANIMOTO



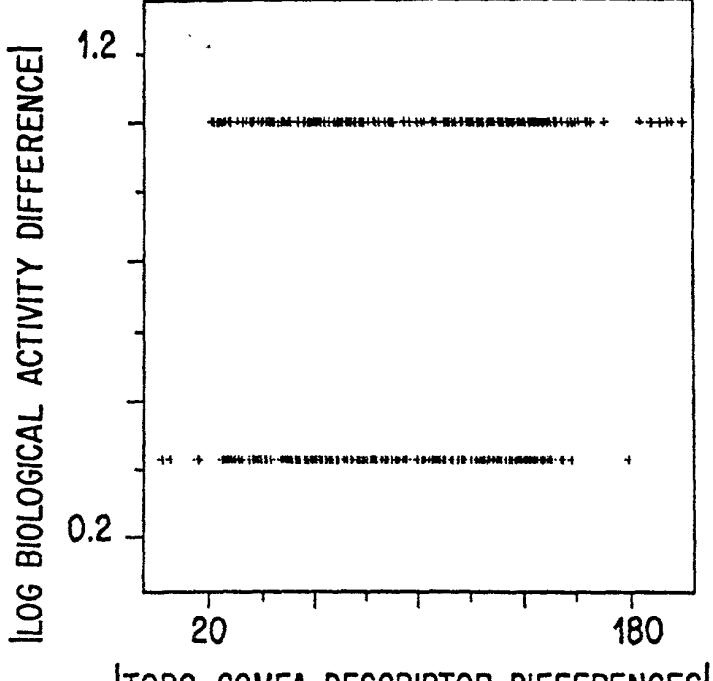


FIG.10(a)

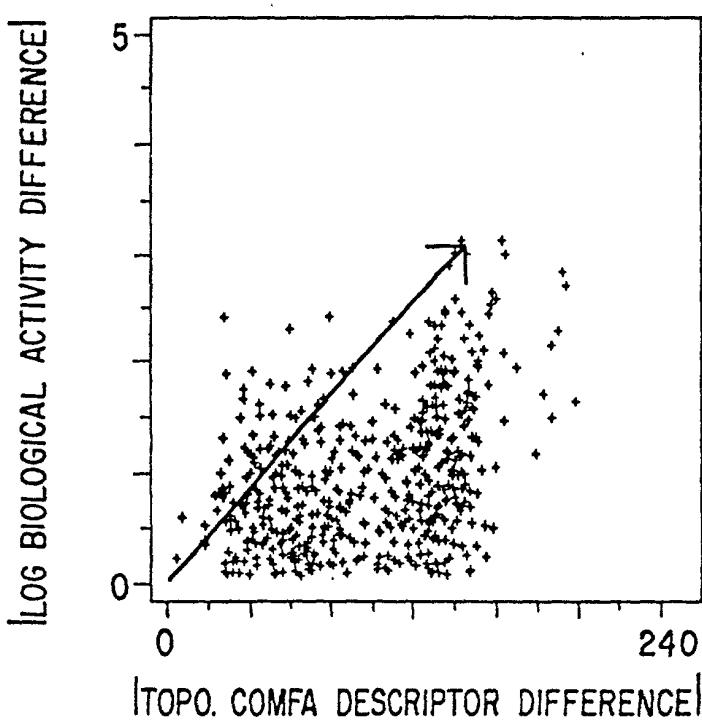


FIG.10(b)

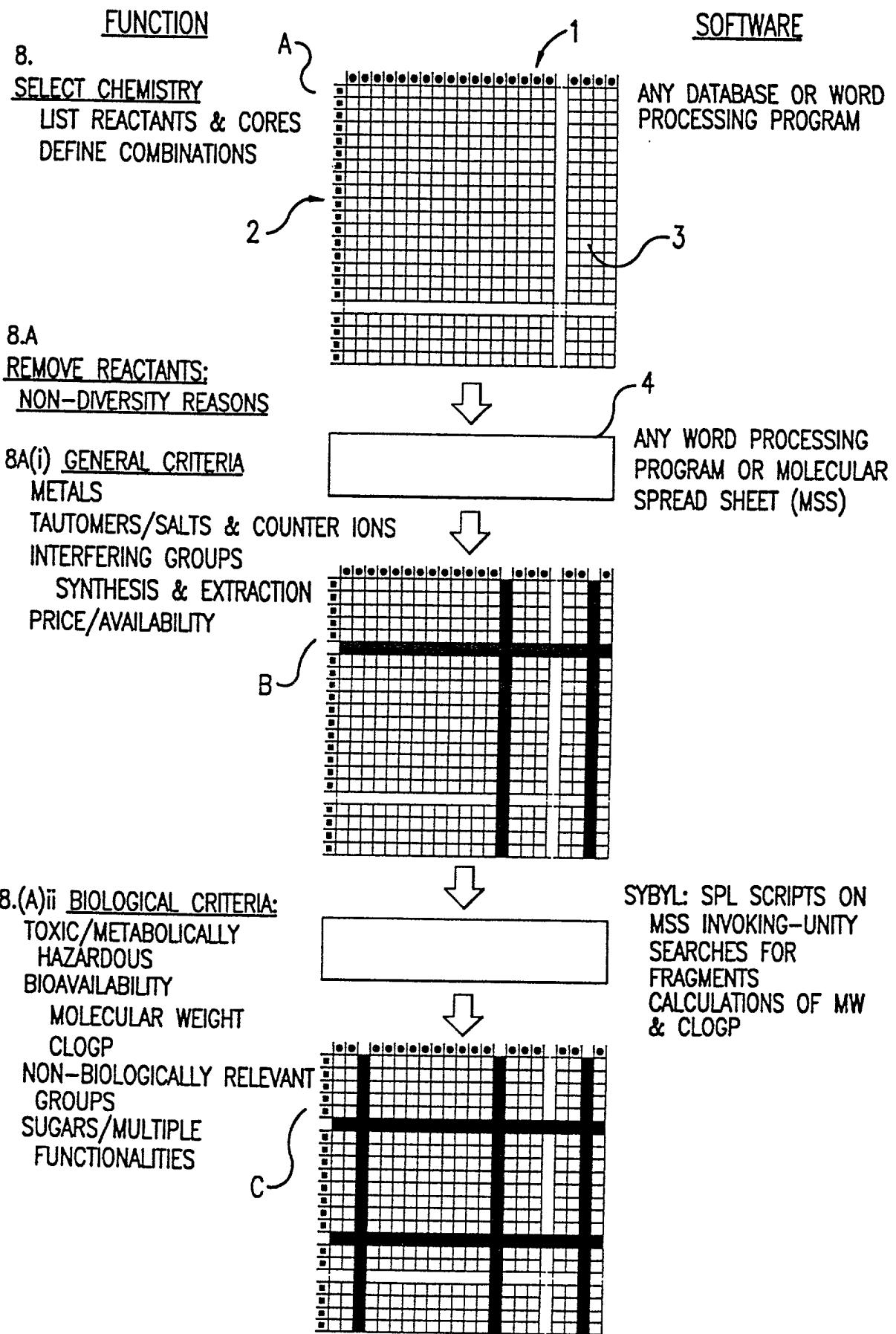


FIG.11(a)

8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION

TOPOMERIC CONFORMER ALIGNMENT

REFINEMENT CoMFA FIELD GENERATION

HYDROGEN BOND FIELD GENERATION

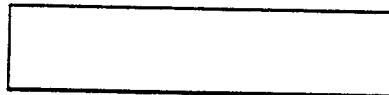
GENERATION
ROTATABLE BOND FIELD
ATTENUATION

ATTENUATION CALCULATE FIELD

DIFFERENCES CLUSTER

CLUSTER SPACES

REACTANT SELECTION FROM EACH CLUSTER



**SYBYL: SELECTOR &
CONCORD 3.2.1
SPECIALIZED SOFTWARE:
APPENDIX "A"
(SYBYL: CoMFA
STERIC & MSS)**

SYBYL: HIERCHICAL
CLUSTER - MSS
SYLBL: MSS

8C

COMBINE REACTANTS TO BUILD PRODUCTS

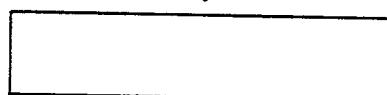


SYBYL: LEGION MSS

8D

REMOVE PRODUCTS:

GENERAL CRITERIA-



SYBYL: SPL SCRIPTS ON MSS

E

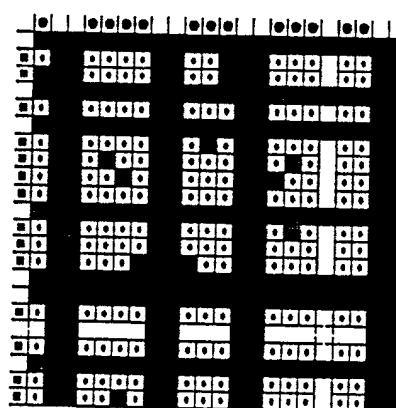
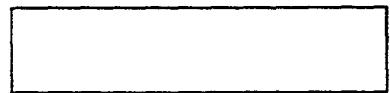


FIG.11(b)

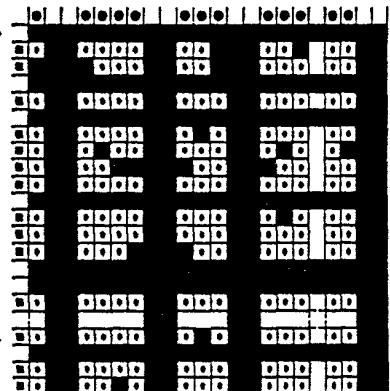
8D

BIOLOGICAL CRITERIA:
METABOLICALLY HAZARDOUS
BIOAVAILABILITY
MOLECULAR WEIGHT
CLOGP



SYBYL: SPL SCRIPTS ON
MSS INVOKING -
UNITY SEARCHES FOR
FRAGMENTS
CALCULATIONS OF MW
& CLOGP

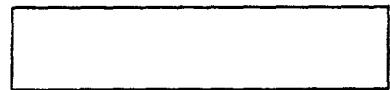
G



8E

REMOVE NON-DIVERSE
PRODUCTS:

GENERATE TANIMOTO
2D FINGERPRINTS
SAMPLE PRODUCTS:
EXCLUDE TAN \geq 0.85



UNITY

H

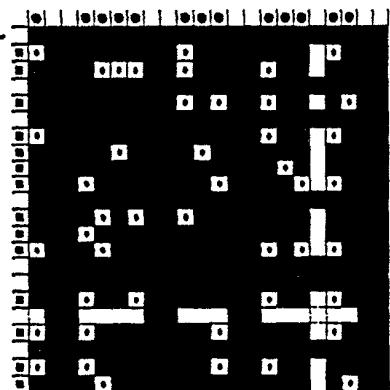


FIG.11(c)

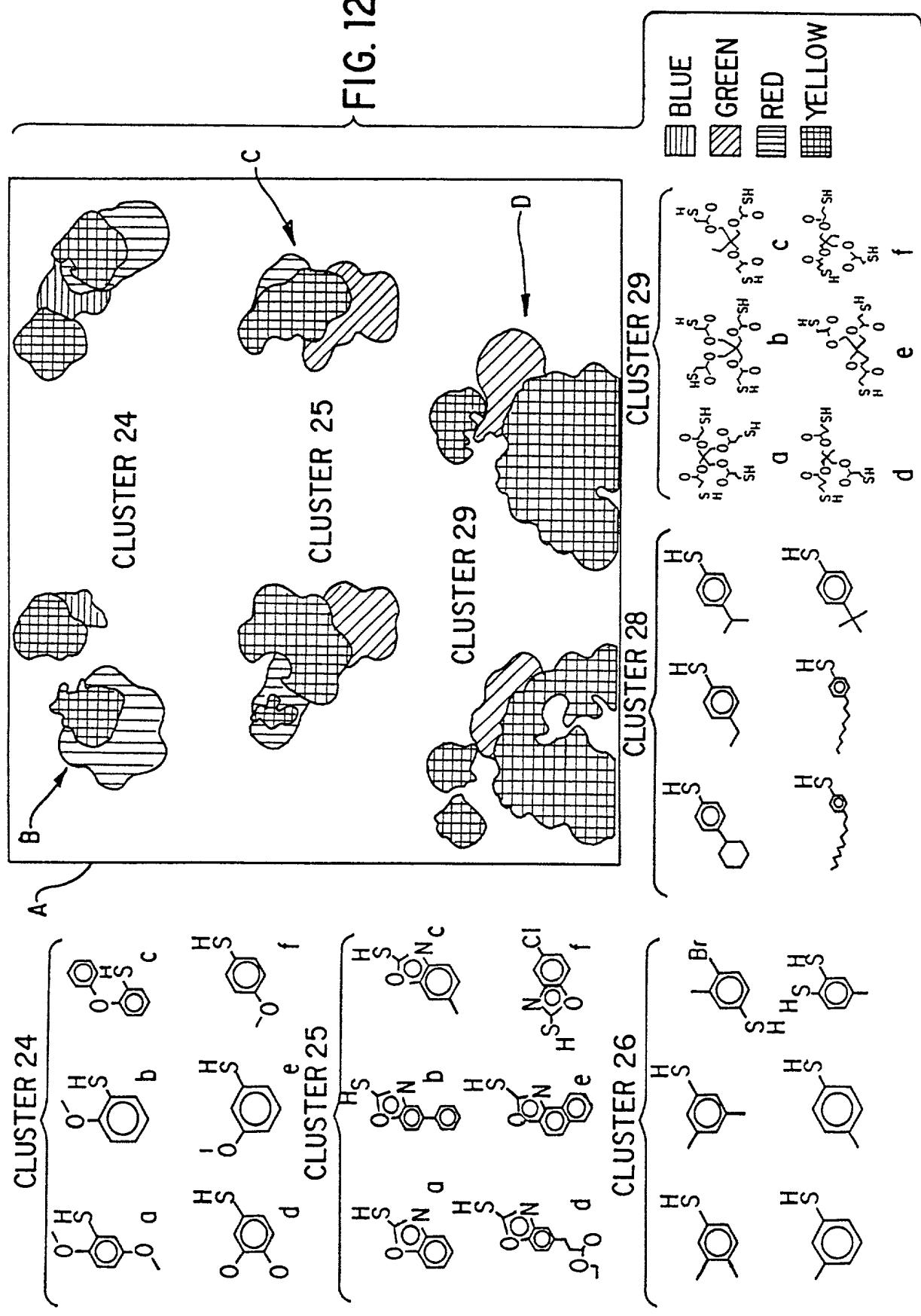
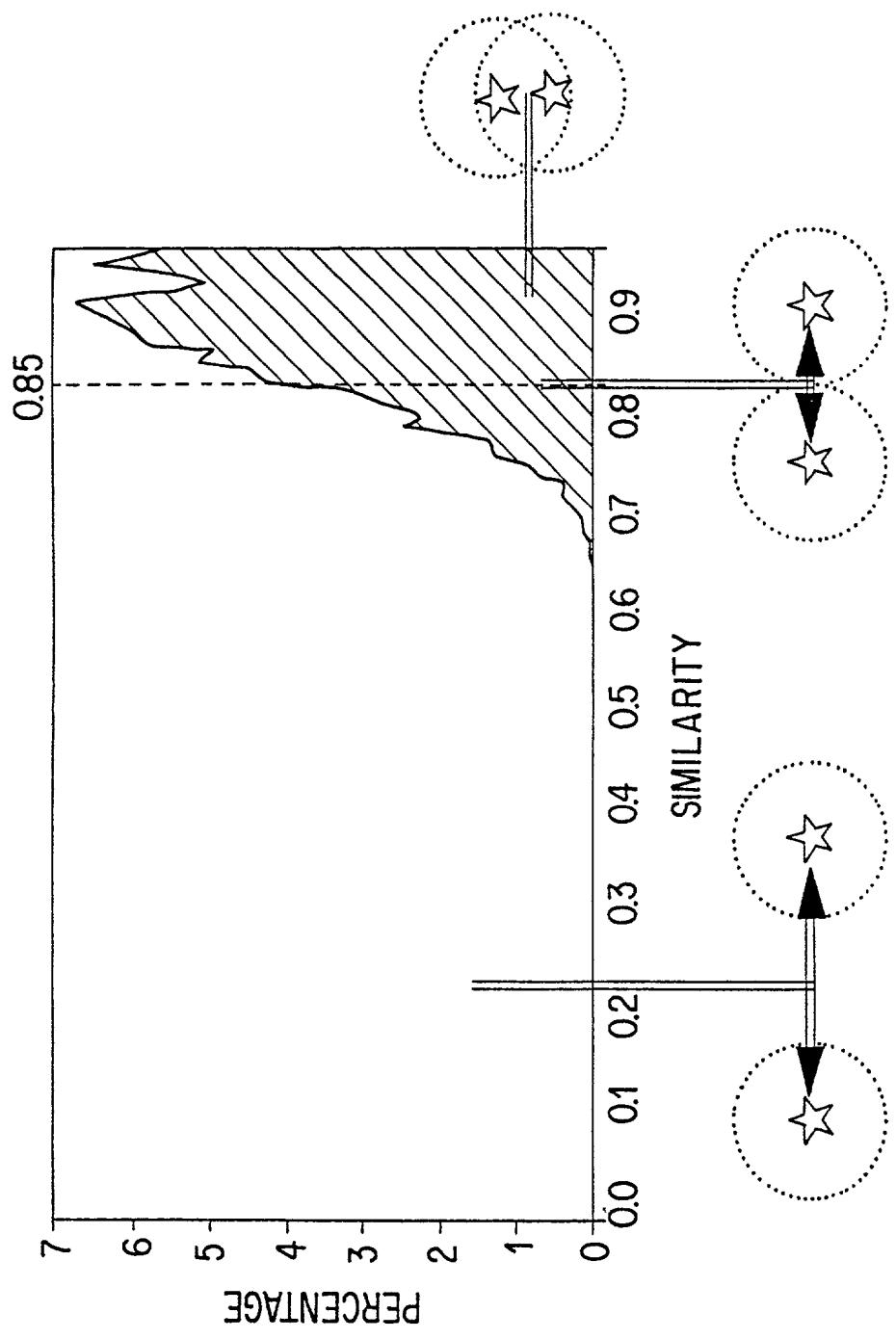


FIG. 13



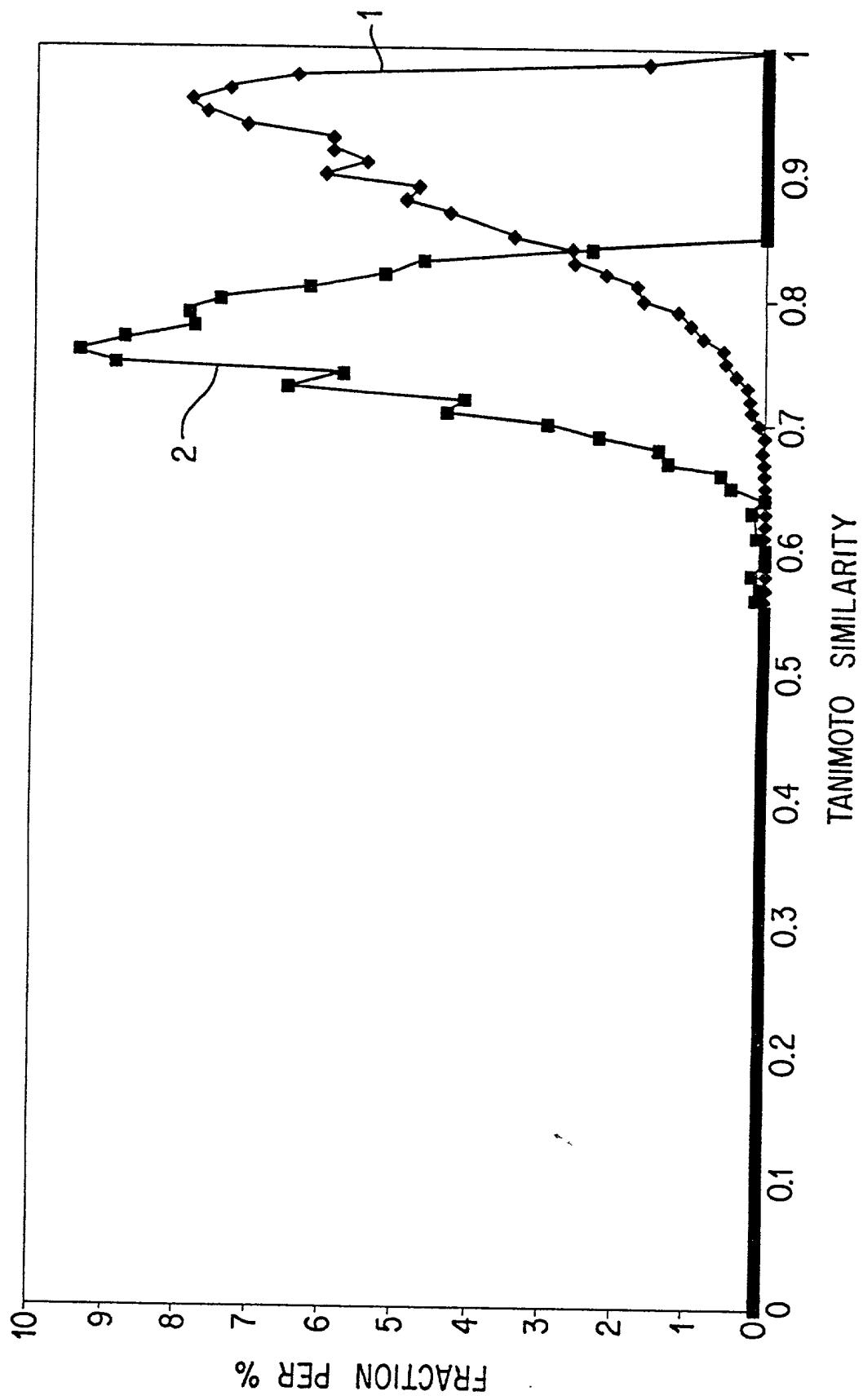


FIG. 14

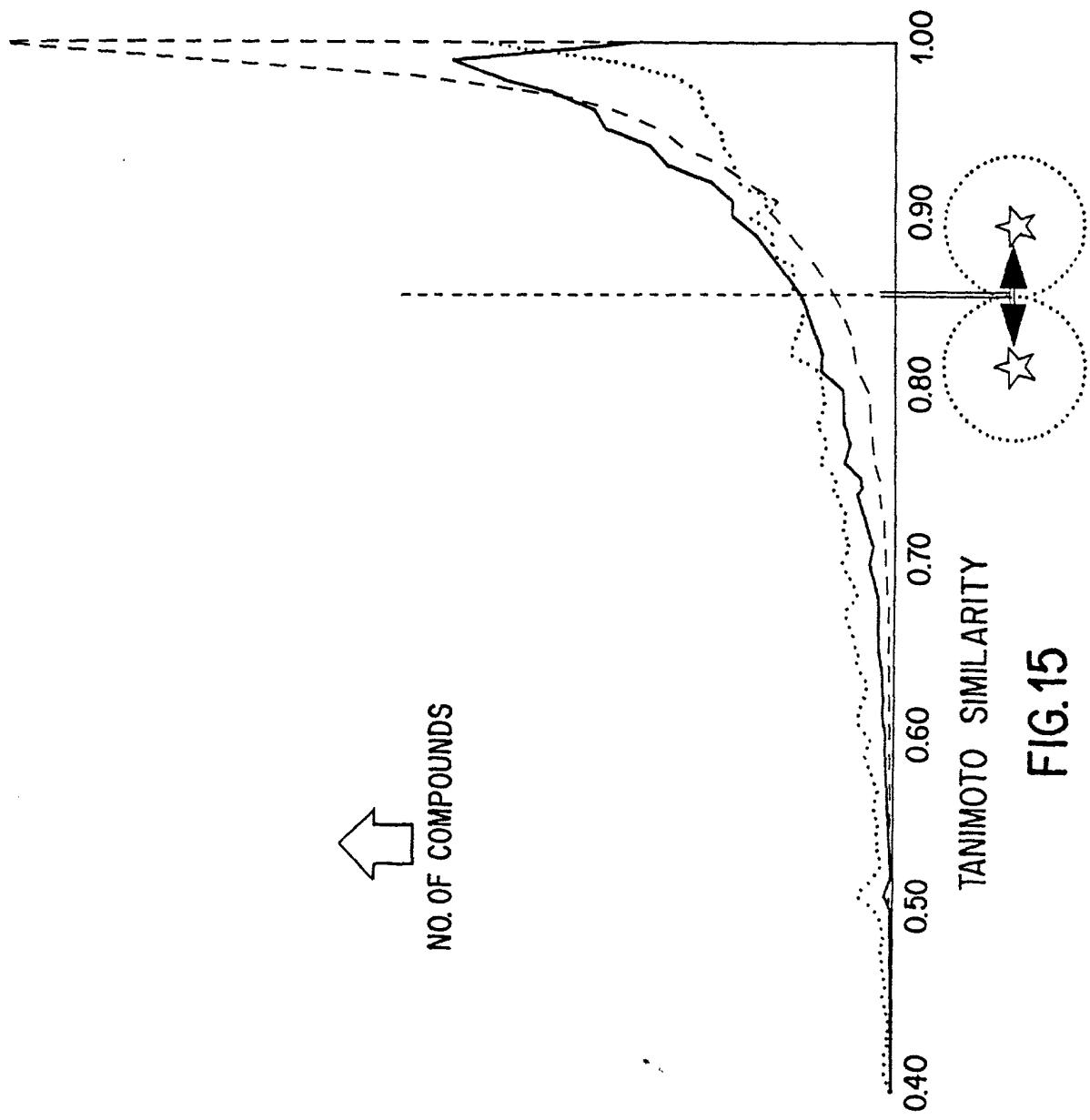


FIG. 15